High Energy and Momentum Resolved Photoemission Studies of Quasi-One-Dimensional Blue Bronze $K_{0.3}MoO_3$

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Why are we interested in
high energy and momentum resolution?
What are the goals?

Nesting properties of the Fermi surfaces
/Charge density waves/

Photoemission spectral functions A(k,w)
/direct comparison with theoretical predictions/

Outline

Experimental details:

- ✓ **Photoelectron spectrometer**

Introduction to $K_{0.3}MoO_3$:

- ✓ **Crystal structure**
- ✓ **Electronic structure**
- ✓ **Structural studies /Charge Density Waves/**

Experimental data:

- ✓ **Band structure of $K_{0.3}MoO_3$**
- ✓ **Fermi wave vectors versus temperature**
- ✓ **Incommensurate to commensurate CDW transition**
- ✓ **Signatures of non-Fermi liquid behavior**

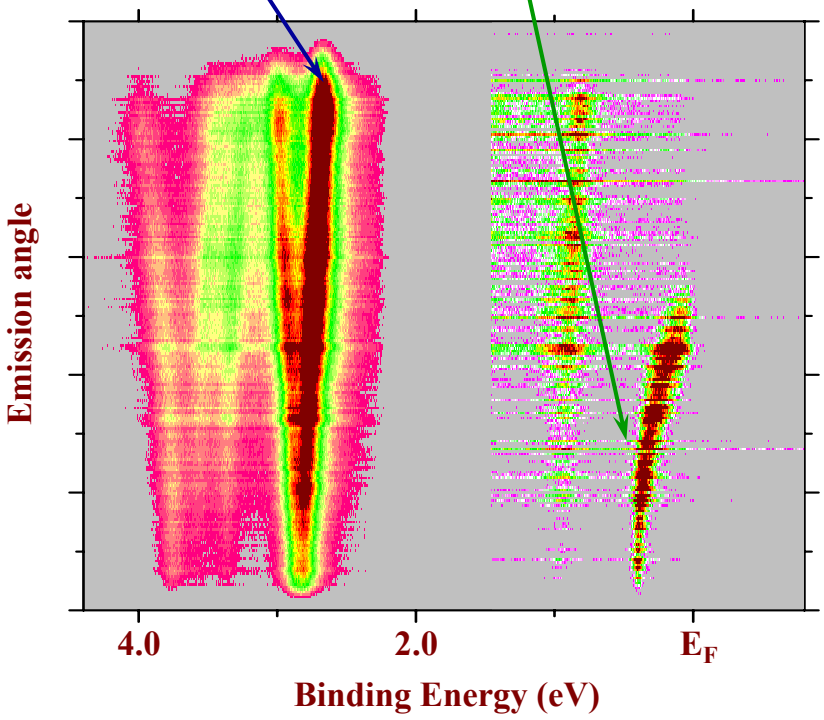
Photoelectron Spectrometer

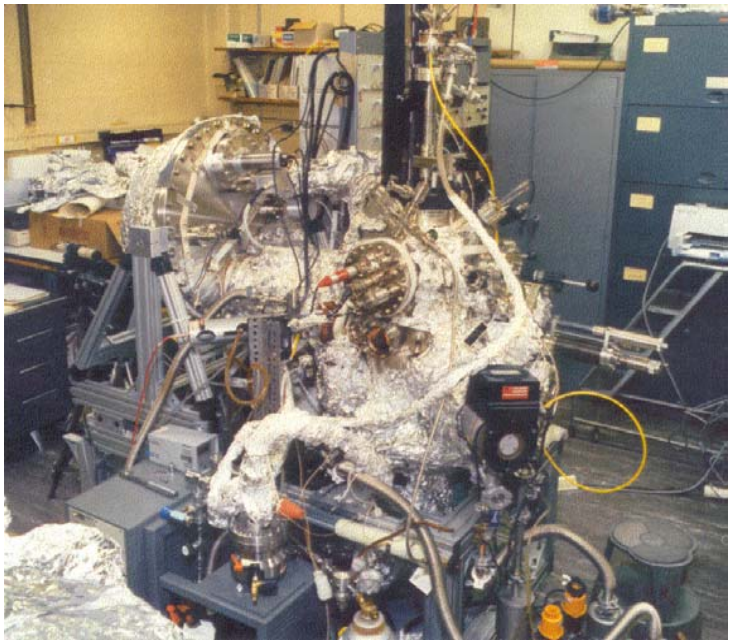
SES-200: 200 millimeters hemispherical deflector capable of multichannel detection in emission angle and kinetic energy

Example of angle resolved data:

hν = 21.22 eV /He I radiation/

Cu(111), bulk bands and sp surface state



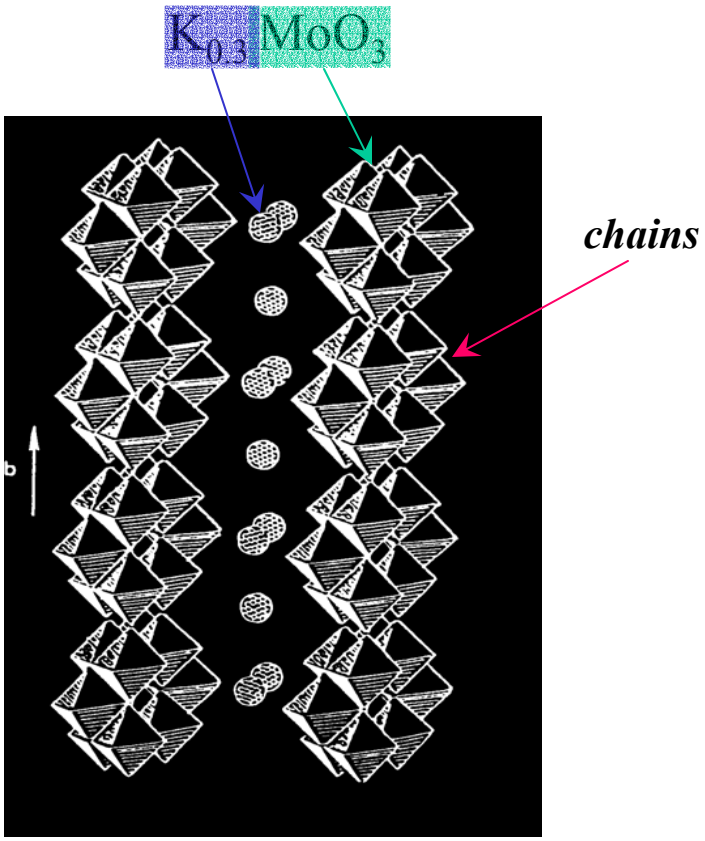


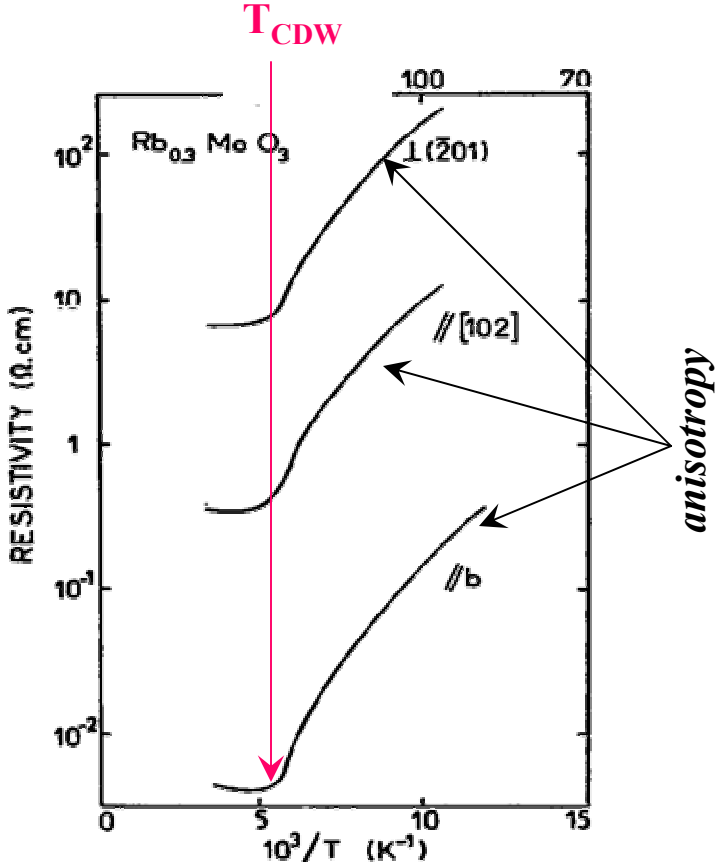
- ✓ *Energy resolution ~ 10 meV*
- ✓ *Angle resolution ~ 0.2 ^{o}*
- ✓ *Base pressure ~ 2× 10^{-11} Torr*

Presently located at the undulator beamline U13UB at the National Synchrotron Light Source

Low dimensionality ⇒

Charge Density Waves (CDW) /Peierls transitions /
Electron correlation effects
/non-Fermi liquid behavior, spin-charge separation, HTSC/





J.-P. Pouget et al., J. Physique Lett. 44, L113 (1973)

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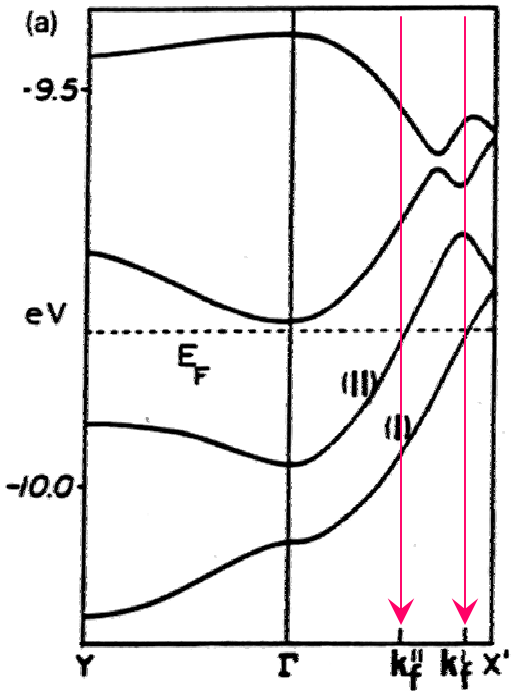
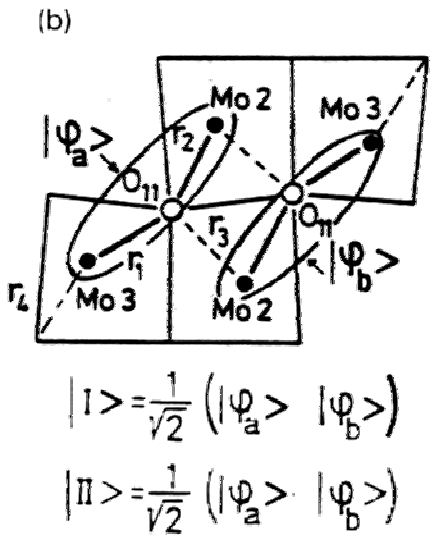
Electronic structure of $K_{0.3}MoO_3$

/tight-binding calculations/

M.-H. Whangbo and L.F. Schneemeyer, Inor. Chem. 25,2424 (1986)





$$|I> = \frac{1}{\sqrt{2}}\left(|\varphi_a> \; |\varphi_b>\right)$$

$$|II> = \frac{1}{\sqrt{2}}\left(|\varphi_a> \; |\varphi_b>\right)$$

Two bands crossing the Fermi level

How many Charge Density Waves?

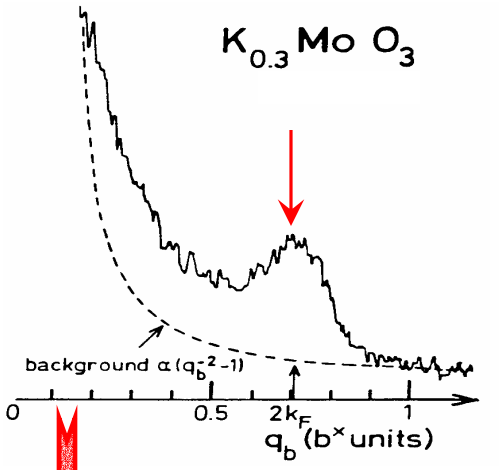
Structural studies of $K_{0.3}MoO_3$

/Single Charge Density Wave/

(i) Diffuse X-ray scattering

$/q_{CDW} = 2k_F b^x/$

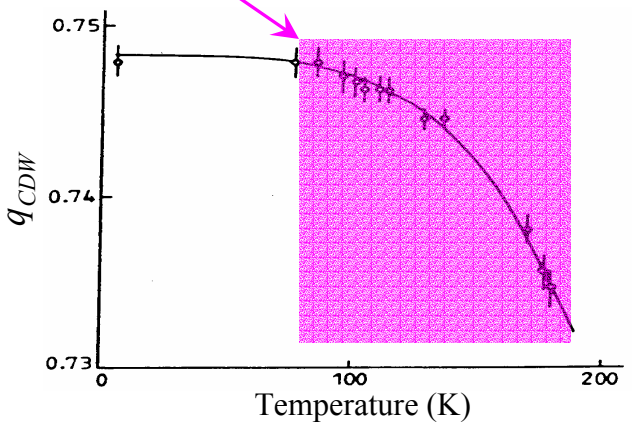
J.-P. Pougetet al.



(ii) Temperature dependent neutron scattering

/ incommensurate to commensurate transition/

M.Sato, H. Fujishita and S.Hoshito,
J. Phys. C: Solid State phys., 16, L877 (1983)

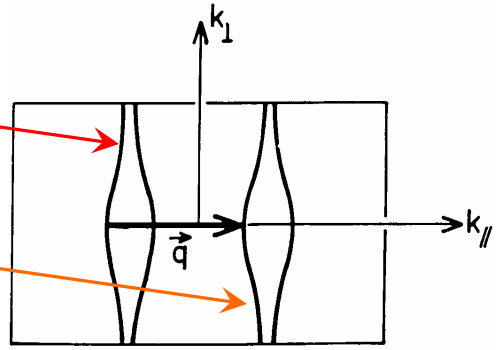


Nesting:

Fermi surface of the first band

is nested to the Fermi surface

of the second band



CDW wave vector

$q_{CDW} : k_{F1}+k_{F2}$

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Temperature dependence of CDW wave vector:

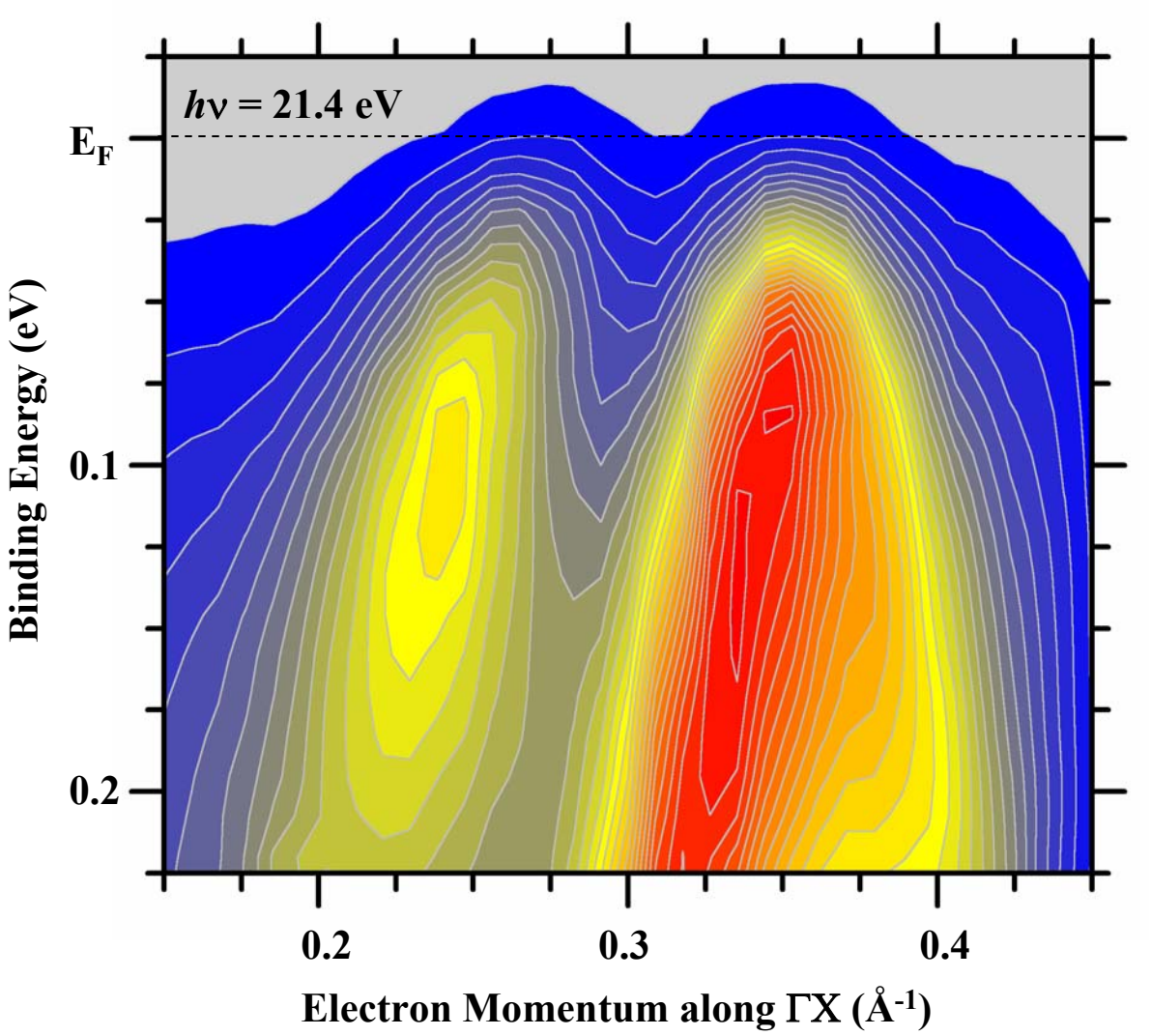
- Thermally activated charge transfer between bands crossing the Fermi level and third band above it */Pouget et al./*
- Shift of the chemical potential */Pouget & Nougera, Artemenko et al./*
- Hidden temperature dependence of the nesting vector */Intention of the present study/*

Goals of photoemission experiment:

- Direct monitoring k_{F1} and k_{F2}
- Temperature dependence of $(k_{F1}+k_{F2})$

Direct monitoring electron bands in $K_{0.3}MoO_3$

/3-D maps of photocurrent/



Experimental details:

Samples cleaved *in situ*

Liquid He cryostat provides temperatures from ~20 K to ~450 K

Temperature monitored with a help of OMEGA CY7 sensor

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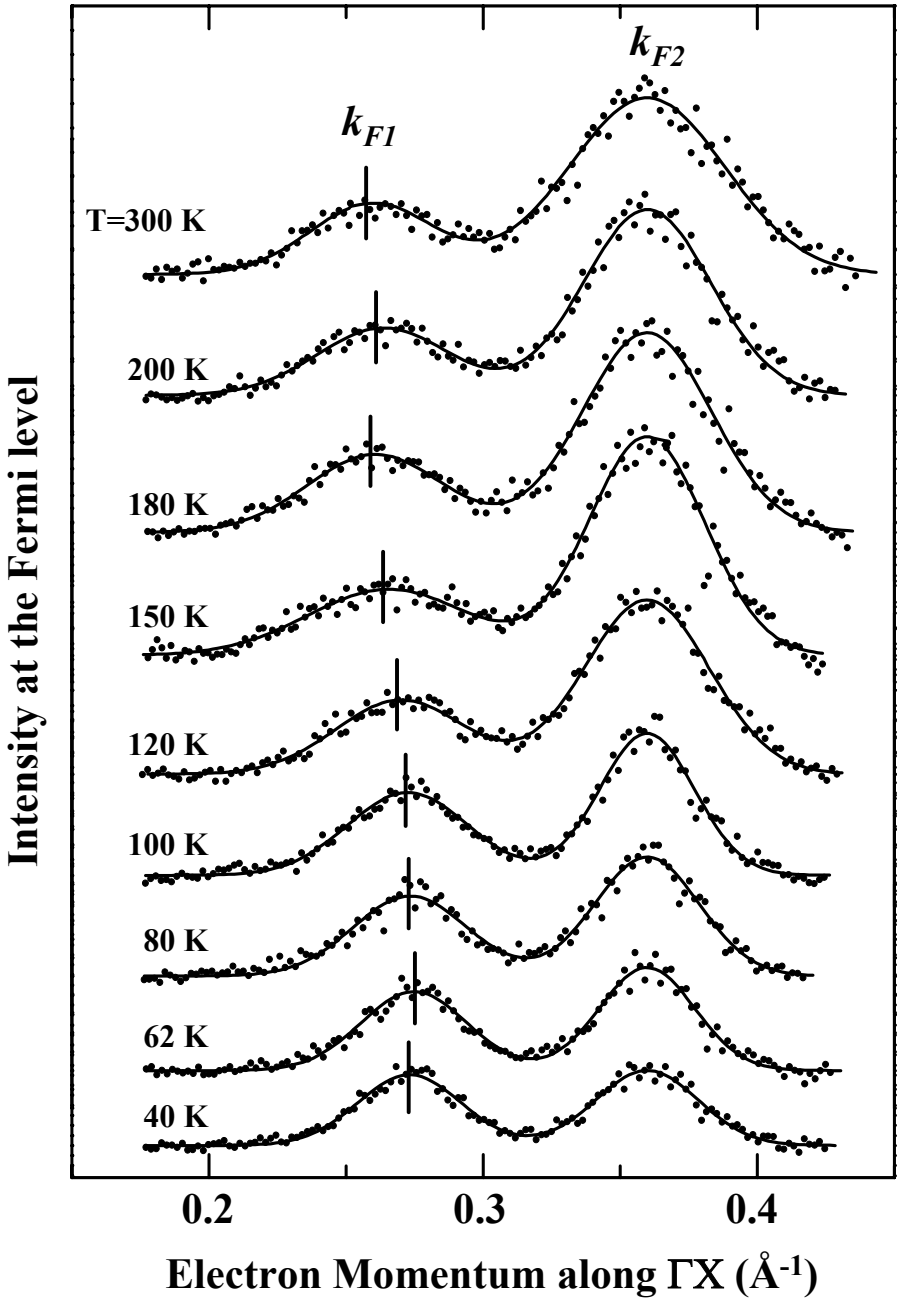
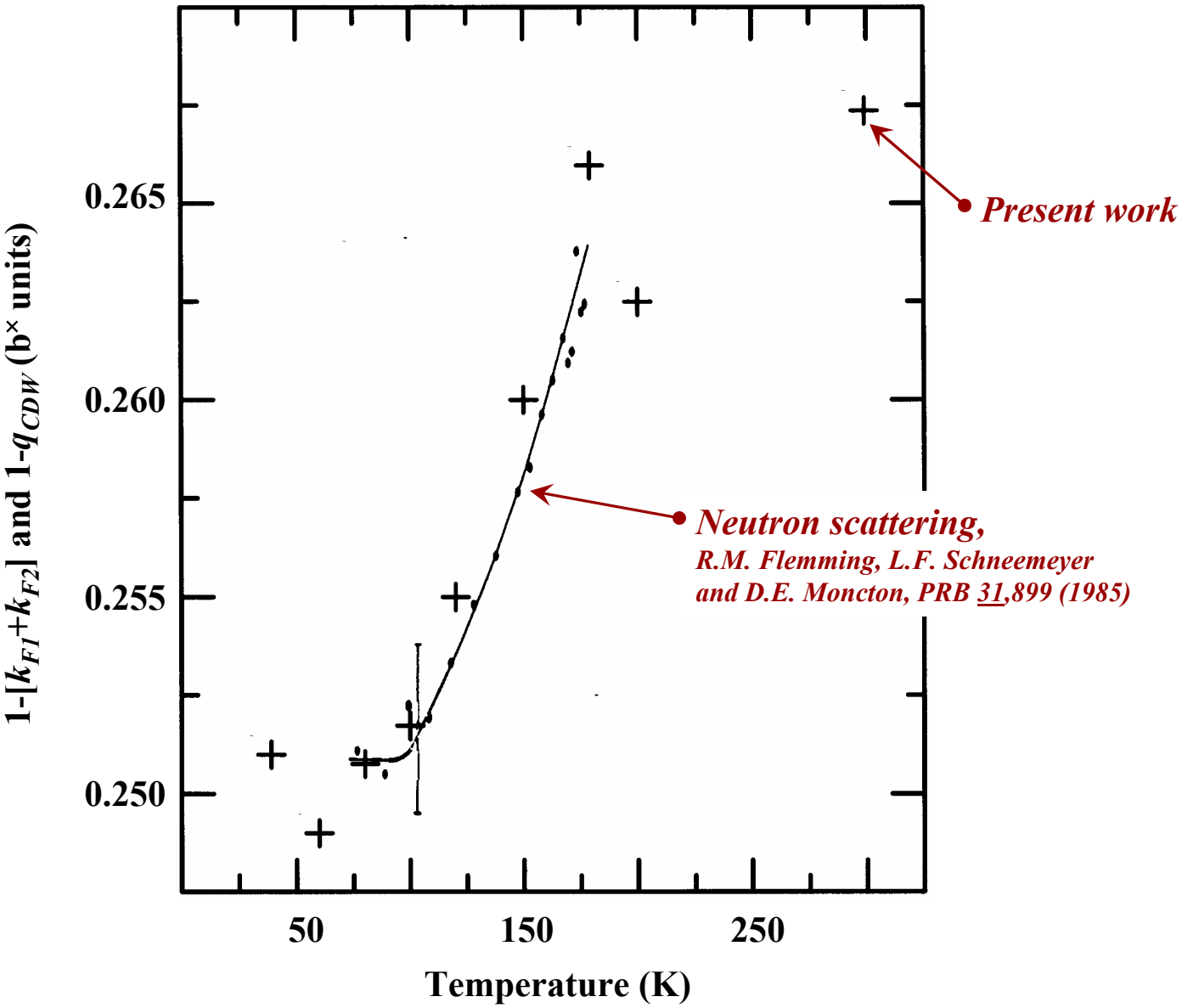
Momentum Distribution Curves at E_F



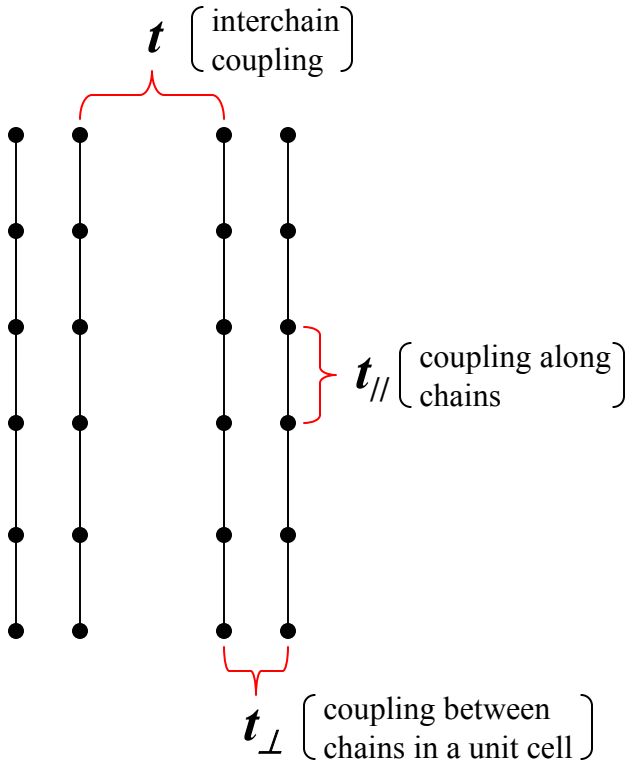
Incommensurate to commensurate CDW transition in $K_{0.3}MoO_3$

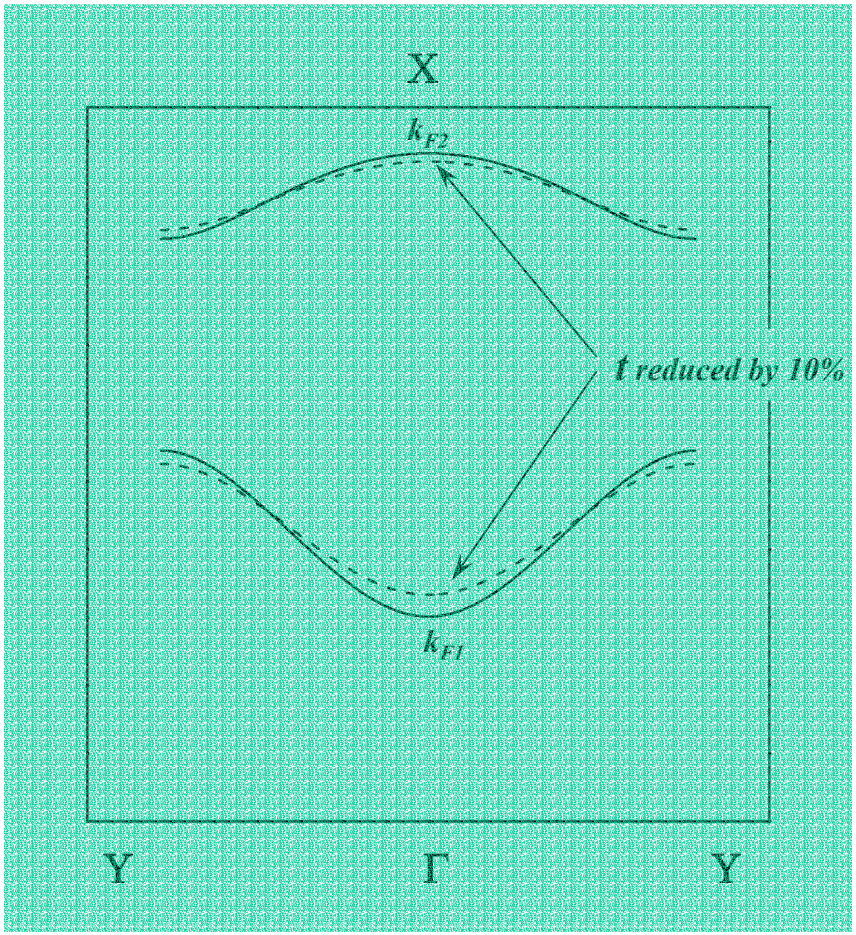
/comparing neutron scattering data with nesting vector measured in photoemission experiment/



Fermi surface of an array of coupled chains

/tight binding calculation/





Fermi surface is given by:

$$\mu = -2\cos(k_{//}) \pm (t_{\perp} + 2t_{\perp}\, t\cos(k_{\perp}) + t)$$

What are the signatures of non-Fermi liquid behavior in photoemission?

Spin-charge separation $\Rightarrow$ **Observation of two dispersing features corresponding to the charge and spin degrees of freedom**

Breakdown of the quasiparticle picture $\Rightarrow$ **Suppression of the spectral weight at the Fermi energy**

PHYSICAL REVIEW B VOLUME 54, NUMBER 18 1 NOVEMBER 1996-II

RAPID COMMUNICATIO

Non-Fermi-liquid behavior due to short-range order

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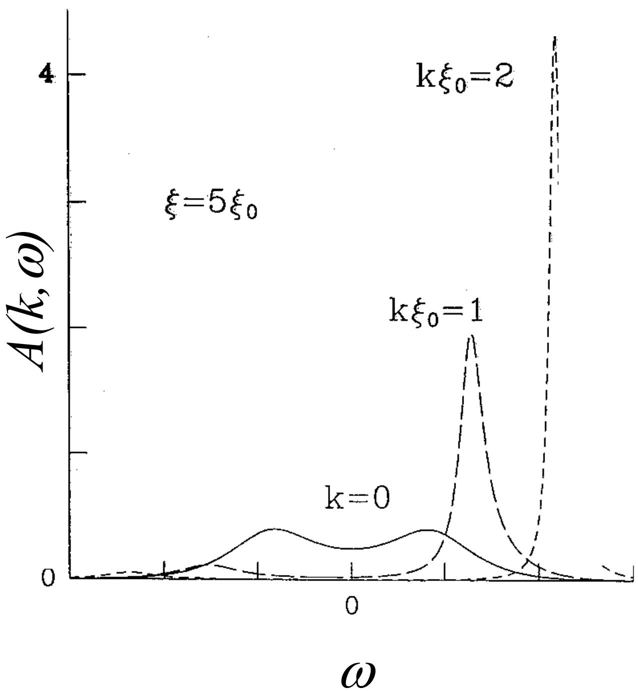
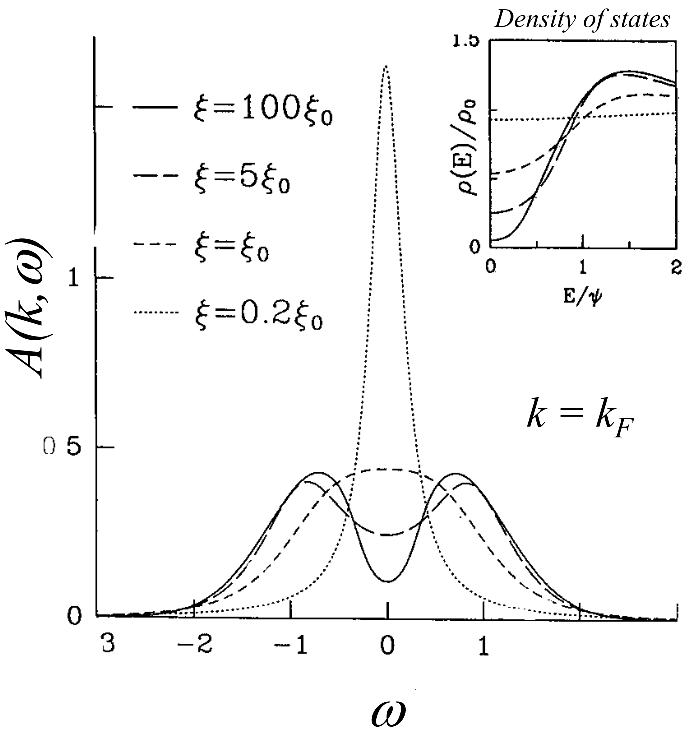
School of Physics, University of New South Wales, Sydney 2052, Australia

(Received 23 May 1996)





J. Phys.: Condens. Matter 5 (1993) 8305–8336. Printed in the UK

Charge–spin separation and the spectral properties of Luttinger liquids

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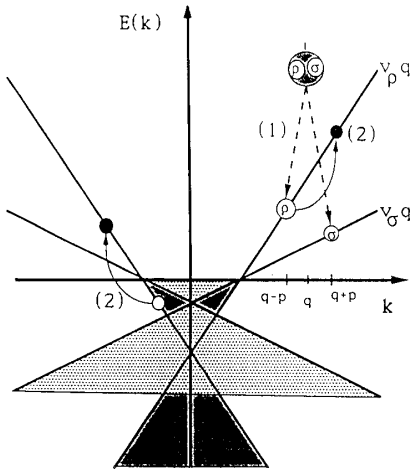
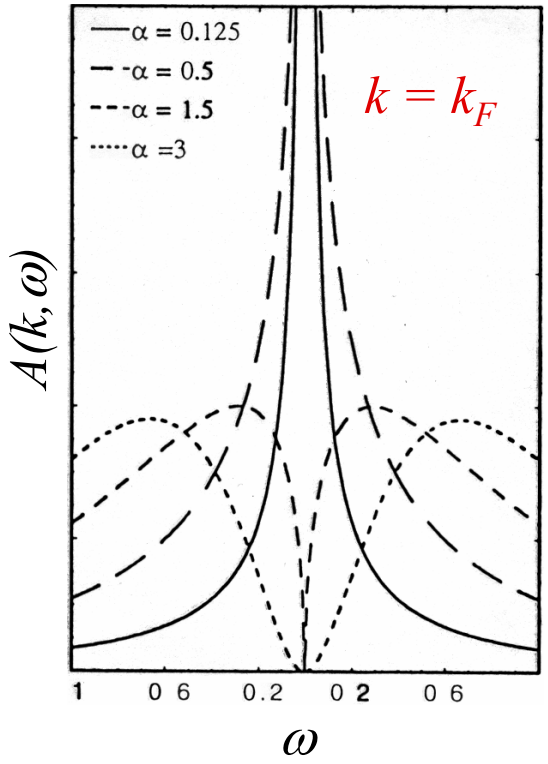
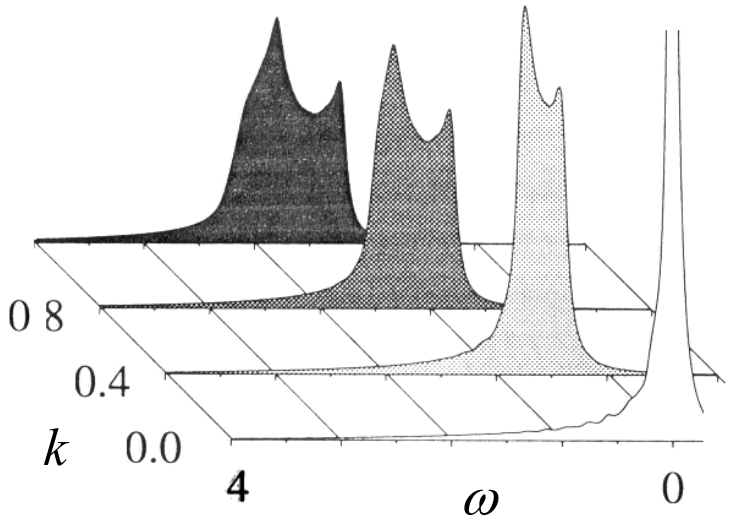


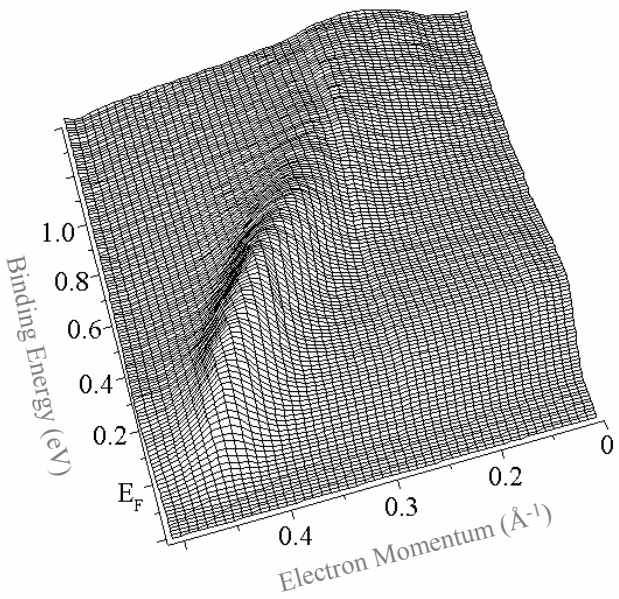


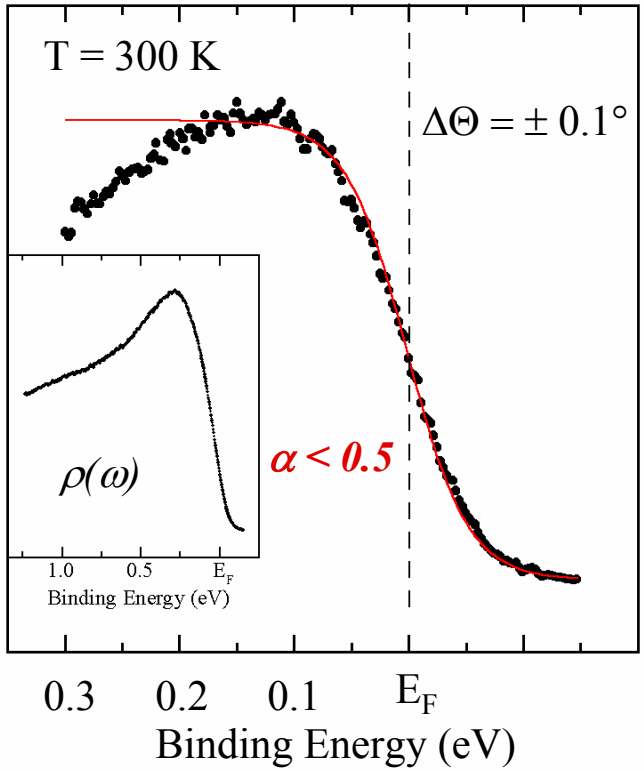
Anomalous Scaling and Spin-Charge Separation in Coupled Chains

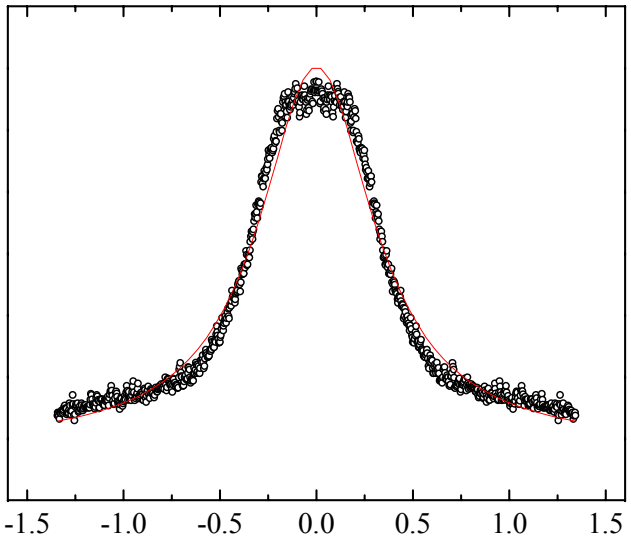
Peter Kopietz, Volker Meden, and Kurt Schönhammer
Institut für Theoretische Physik der Universität Göttingen, Bunsenstrasse 9, D-37073 Göttingen, Germany
(Received 19 August 1994)



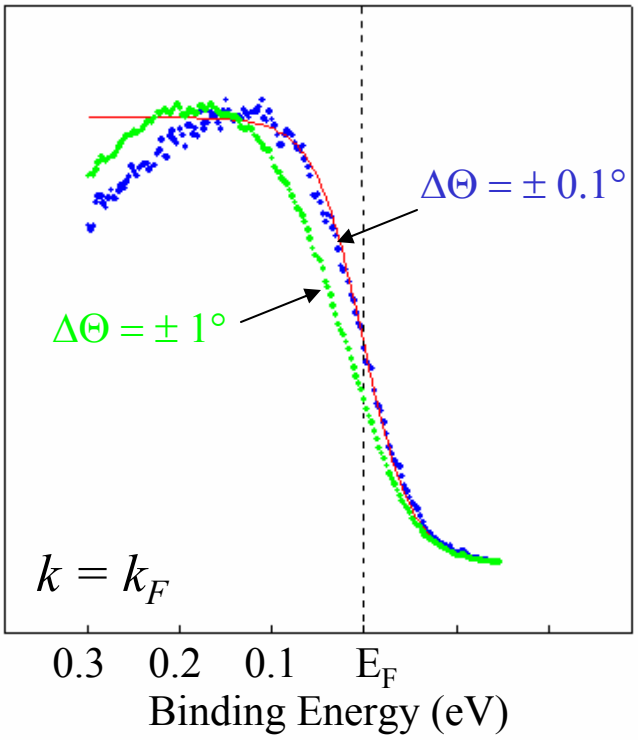
Spectral function in $K_{0.3}MoO_3$ at the Fermi wave vector



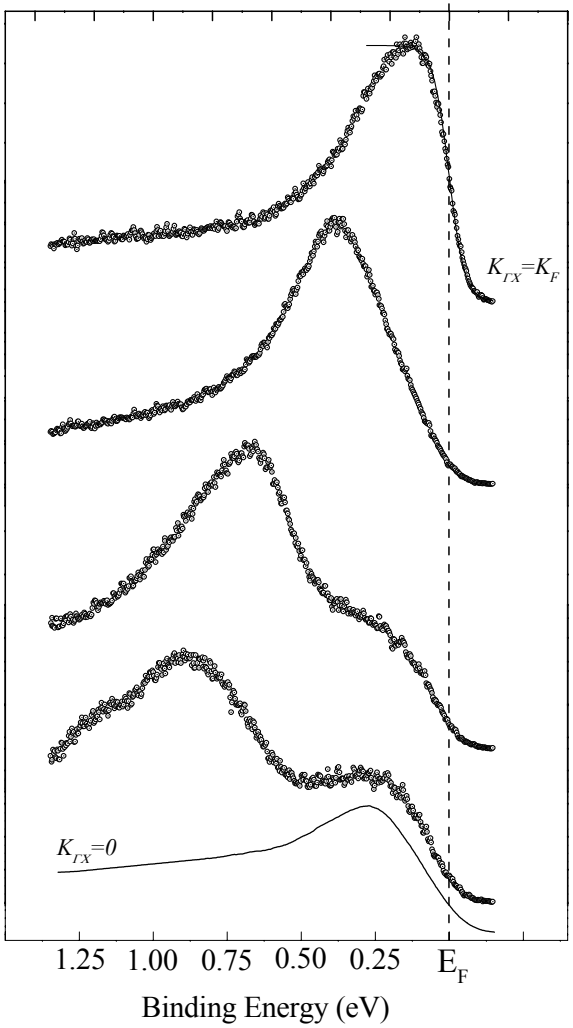


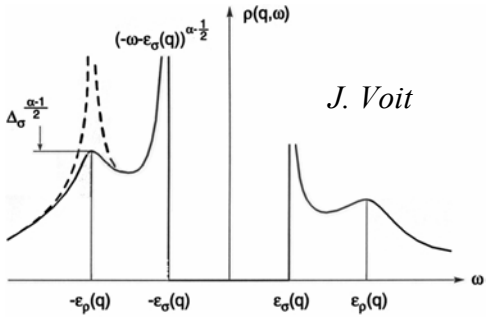

-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5

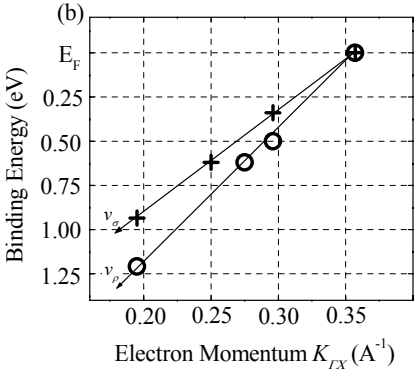
Suppression of spectral weight in photoemission from low-dimensional conductors: influence of momentum resolution



Spectral line-shapes versus electron momentum







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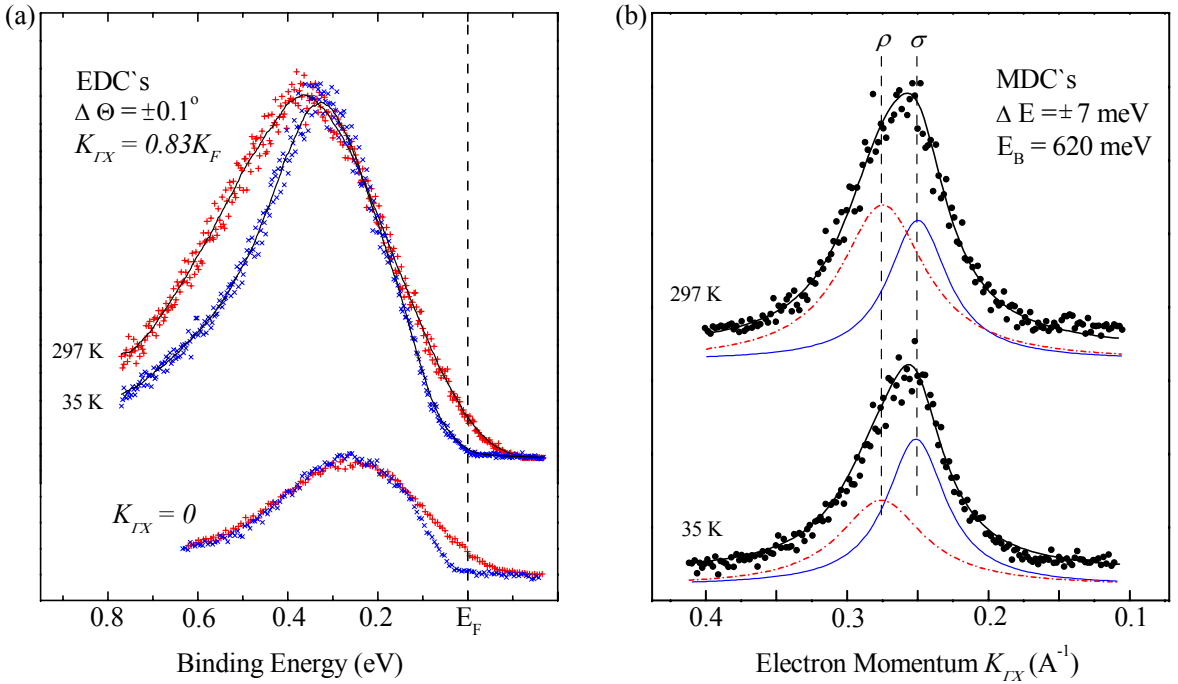
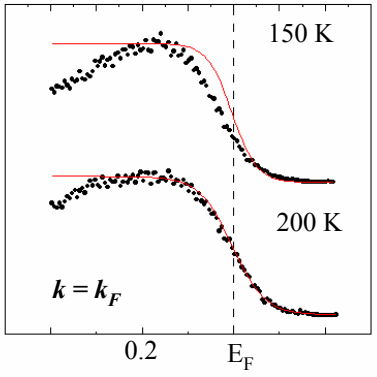
Spectral line-shapes versus temperature





Gap opening at the Fermi wave vector